

# Exact ground state of the Shastry-Sutherland lattice with classical Heisenberg spins

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An exact analytical solution of the ground state problem of the isotropic classical Heisenberg model on the Shastry-Sutherland lattice in external magnetic field  $H$  is found for arbitrary ratio of diagonal and edge exchange constants  $J_2/J_1$ . The phase diagram of this model in the  $(J_2/J_1, H/J_1)$  plane is presented. It includes spin-flop, spin-flip and umbrella phases. The magnetization curves are found to be linear until saturation. It is shown numerically that the inclusion of the easy-axis anisotropy into the model leads to the appearance of the  $1/3$  magnetization plateau, corresponding to the collinear up-up-down spin structure. This explains the appearance of the  $1/3$  magnetization plateau in rare earth tetraborides  $RB_4$ . In particular, magnetization curve of the compound  $HoB_4$  is explained.

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## I. INTRODUCTION

Shastry-Sutherland lattice (SSL) was first introduced in the work of Shastry and Sutherland<sup>1</sup> as a purely theoretical example of a two-dimensional frustrated spin system. SSL is a square lattice with classical Heisenberg, quantum Heisenberg, or Ising spin  $\mathbf{S}_i$  at every lattice site  $i$ , with antiferromagnetic (AFM) exchange  $J_1$  along the edges, and AFM exchange  $J_2$  along certain diagonals, as shown in Fig. 1. Its Hamiltonian (in the presence of the external field  $H$  directed along the  $z$ -axis) is

$$\mathcal{H} = J_1 \sum_{edges} \mathbf{S}_i \mathbf{S}_j + J_2 \sum_{diagonal} \mathbf{S}_i \mathbf{S}_j - H \sum_i S_i^z, \quad (1)$$

and the Hamiltonian normalized by  $J_1$  is

$$\tilde{\mathcal{H}} \equiv \frac{\mathcal{H}}{J_1} = \sum_{edges} \mathbf{S}_i \mathbf{S}_j + \rho \sum_{diagonal} \mathbf{S}_i \mathbf{S}_j - h \sum_i S_i^z, \quad (2)$$

where we have introduced the notations

$$\rho \equiv \frac{J_2}{J_1}, \quad h \equiv \frac{H}{J_1}. \quad (3)$$

Surprisingly, ten years after the work of Shastry and Sutherland, SSL has been experimentally realized in  $SrCu_2(BO_3)_2$ <sup>2</sup>, which has a layered structure, with each  $Cu^{2+}$  ion carrying spin  $S = 1/2$ . If exchange interactions with only two spheres of nearest neighbors are included, the magnetic lattice of  $SrCu_2(BO_3)_2$  is equivalent to SSL. At low temperatures  $SrCu_2(BO_3)_2$  exhibits a sequence of magnetization plateaus at fractional values of the saturation magnetization  $M_s$ <sup>3-5</sup>. A number of theories of this phenomenon has been proposed<sup>6-8</sup>.

Similar fractional magnetization plateaus have been observed recently in rare earth tetraborides<sup>9-12</sup>  $RB_4$ , where  $R = Tm, Er$  or  $Ho$ , where the rare earth ions also form layered structure equivalent to SSL. The important difference is that while  $Cu^{2+}$  ions in  $SrCu_2(BO_3)_2$  have spins  $s = 1/2$ , the rare earth ions in  $RB_4$  systems have

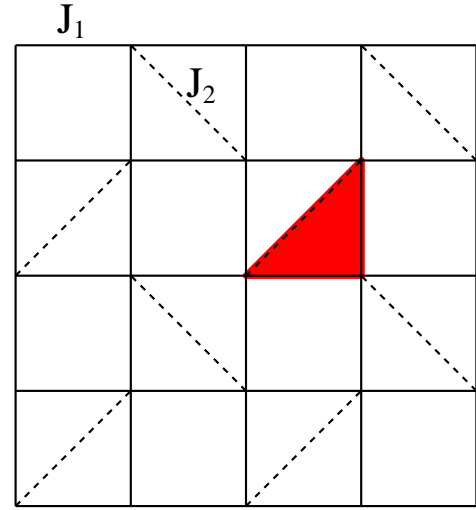


FIG. 1. (Color online) Shastry-Sutherland lattice. The red (gray) triangle marks the elementary cluster of the SSL.

large spins, which can be treated as classical ones. These compounds also possess a strong easy-axis magnetocrystalline anisotropy.

The discovery of magnetization plateaus in  $RB_4$  compounds led to a number of theoretical and computational studies of SSL with classical Heisenberg<sup>13-15</sup> and Ising<sup>16-21</sup> spins. Deep understanding of these two models is vital for explaining the peculiar magnetization curves of  $RB_4$  systems, as they can serve as the foundation stones on which more complicated models with additional interactions can be built. A major breakthrough for Ising SSL in external magnetic field came very recently as its exact ground state has been found analytically<sup>19</sup>. This model gives a single  $M/M_s = 1/3$  magnetization plateau, which corresponds to the so-called up-up-down (UUD) phase (Fig. 2, lower left). On the other hand, a Monte Carlo simulation for the classical Heisenberg SSL<sup>13</sup> found magnetization curves with no steps. However, when the easy-axis anisotropy was included in the

model<sup>14,15</sup>, the  $1/3$  UUD plateau appeared for a certain range of  $J_2/J_1$ . Magnetization steps other than  $1/3$  do not appear for either Ising or Heisenberg SSL. Additional exchange or dipolar interactions<sup>16,19,21</sup> or lattice disorder<sup>14</sup> were employed to account for those plateaus. If these additional interactions are included, Ising model on SSL essentially succeeds in explaining the appearance of fractional magnetization plateaus in  $\text{RB}_4$ . A typical zero-temperature magnetization curve  $M(H)$  of the Ising SSL has the "staircase" shape, namely it consists of horizontal magnetization steps (including the  $M = 0$  and  $M = M_s$  ones) separated by first-order phase transitions (vertical segments of the  $M(H)$  curve). This is very similar to the experimental  $M(H)$  curve of  $\text{TmB}_4$  (Ref. 11). Anisotropic Heisenberg SSL<sup>14,15</sup>, on the other hand, gives smoother  $M(H)$  curves with inclined regions, which were experimentally observed for  $\text{HoB}_4$  (Ref. 12) and possibly  $\text{ErB}_4$  (Ref. 9).

While the exact ground state of the Ising SSL in magnetic field has been found, the complete understanding of the classical Heisenberg SSL is still lacking. In particular, its exact ground state has not been determined, except for special cases  $H = 0$  (Ref. 1) and  $J_2/J_1 = 2$  (Ref. 13). The Monte Carlo simulations<sup>13–15</sup> mainly focused on the special point  $J_2/J_1 = 2$  or its vicinity, while the phase diagram in the  $(J_2/J_1, H/J_1)$  plane has never been published. The present paper is an attempt to clarify these issues. Its goal is to study in detail the ground-state problem of the isotropic classical Heisenberg SSL and to determine the phase diagram of this model in the  $(\rho, h)$  plane. The very interesting problem of the classical Heisenberg SSL with easy-axis anisotropy is also addressed briefly in the present paper.

The paper is organized as follows. Section II introduces different possible magnetic structures of the SSL and presents its phase diagram in the  $(\rho, h)$  plane. In section III the exact ground state of the SSL is calculated and it is proven that the three phases of the previous section are indeed the ground state spin structures. Section IV checks the exact result with numerical simulation and examines the effect of the uniaxial anisotropy on the magnetization curves. It is followed by a conclusion.

## II. MAGNETIC STRUCTURES AND THE PHASE DIAGRAM

In this and the following sections we consider the problem of the ground state of the SSL as the function of two parameters:  $h \equiv H/J_1$  and  $\rho \equiv J_2/J_1$ . In the absence of external magnetic field ( $h = 0$ ) the problem has been solved in Ref. 1. For  $\rho < 1$  ( $J_2 < J_1$ ) the ground state is the regular Neel AFM state (Fig. 2, upper left) with the energy per lattice site

$$\epsilon_{\text{Neel}} = -2 + \frac{\rho}{2}. \quad (4)$$

The Neel state satisfies all  $J_1$  exchange interactions, but not  $J_2$  ones. For  $\rho > 1$  ( $J_2 > J_1$ ) the ground state is

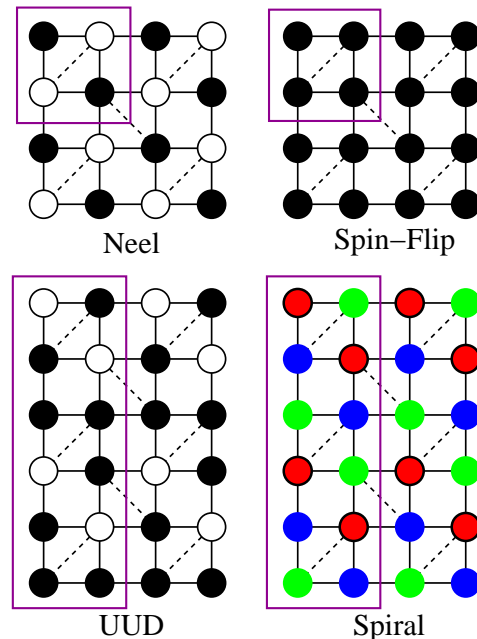


FIG. 2. (Color online) Neel, spin-flip, UUD and spiral (for  $J_2/J_1 = 2$ ) spin structures. Black and white circles denote spins pointing up and down respectively. Red, green and blue circles denote three different directions of the spiral structure, with angle  $120^\circ$  between each two directions. The magnetic unit cells are shown with purple (gray) rectangles.

the so-called spiral state. The angle between neighboring spins is  $\pi - \Delta\phi$  along the edges, and  $2\Delta\phi$  along the diagonals, where  $\Delta\phi = \cos^{-1}(1/\rho) = \cos^{-1}(J_1/J_2)$ . The energy of this structure is

$$\epsilon_{\text{Spiral}} = -\frac{1}{\rho} - \frac{\rho}{2}. \quad (5)$$

Such configuration can be constructed in an infinite number of ways, leading to a degeneracy<sup>1,13</sup>. In general, it is incommensurate with the crystal lattice, but for chosen values of  $\rho$ , namely for  $\cos^{-1}(1/\rho) = \pi m/n$  with integer  $m, n$ , periodic spirals can be realized. One possible spiral configuration for  $\rho = 2$  is presented in Fig. 2, lower right.

The special case  $\rho = 2$  ( $J_2/J_1 = 2$ ) for  $h > 0$  has been solved in Ref. 13. In this case the Hamiltonian (1) possesses an additional degeneracy, and there is an infinite number of spin structures which share both total energy and the magnetization with the umbrella structure introduced below. The generic case  $h > 0$  is a bit more complicated. First we introduce several candidate spin structures which correspond to the local extrema of the total energy and present the phase diagram of the SSL in the  $(\rho, h)$  plane. In the next section we prove rigorously that the three structures considered (spin-flop, spin-flip and umbrella) are indeed the lowest-energy structures in the respective regions of the  $(\rho, h)$  plane.

UUD structure, shown in Fig. 2, has energy and mag-

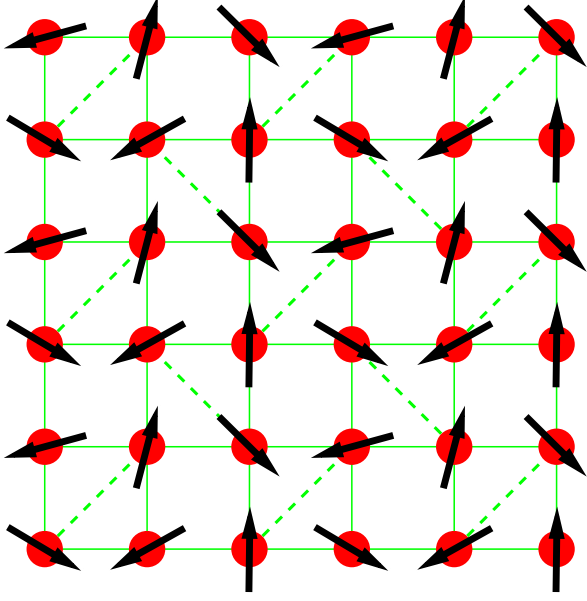


FIG. 3. (Color online) Umbrella structure for  $\rho = 1.5$ ,  $h = 3$  calculated numerically on the  $6 \times 6$  lattice with periodic boundary conditions. The arrows show the  $xy$  components of spins. The red (gray) circles show the  $z$  components of spins (all equal for the umbrella structure).

netization:

$$\epsilon_{UUD} = -\frac{2}{3} - \frac{\rho}{6} - \frac{h}{3}, \quad M_{UUD} = 1/3. \quad (6)$$

Here and in the following we define  $M$  as the magnetization per lattice site, so that  $M_s = 1$ . The spin-flop structure is the Neel structure with all spins tilted by the angle  $\theta' = \pi/2 - \theta = \sin^{-1}(h/8)$  out of the  $xy$  plane. This solution exists for  $h < 8$ , and its energy and magnetization are given by

$$\epsilon_{Flop} = -2 + \frac{\rho}{2} - \frac{h^2}{16}, \quad M_{Flop} = \cos(\theta) = \frac{h}{8}. \quad (7)$$

The spin-flip (ferromagnetic) structure (Fig. 2, upper right) has all spins aligned along the magnetic field. Its energy is

$$\epsilon_{Flip} = 2 + \frac{\rho}{2} - h, \quad M_{Flip} = 1. \quad (8)$$

At  $h = 8$  the spin-flop structure turns into the spin-flip structure in a continuous fashion. Since  $M(h)$  is continuous at the point  $h = 8$ , but  $\partial M(h)/\partial h$  is not, this is a second-order phase transition.

Another possible structure is the umbrella structure, proposed in Ref. 13. It is essentially a tilted spiral structure. In the umbrella structure the spherical angles  $\theta_i$  of all spins are equal, and the angles  $\phi_i$  are distributed like in the spiral structure above. The energy for given  $\theta, \Delta\phi$

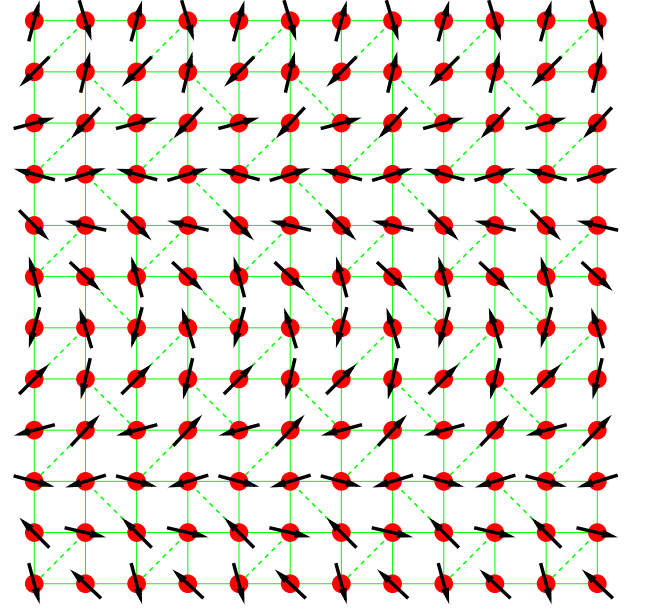


FIG. 4. (Color online) Umbrella structure for  $\rho = 1.5$ ,  $h = 3$  calculated numerically on the  $12 \times 12$  lattice with periodic boundary conditions. The arrows show the  $xy$  components of spins. The red (gray) circles show the  $z$  components of spins (all equal in this case).

is

$$\epsilon(\theta, \Delta\phi) = 2(-\sin^2\theta \cos(\Delta\phi) + \cos^2\theta) + \frac{\rho}{2}(\sin^2\theta \cos(2\Delta\phi) + \cos^2\theta) - h \cos\theta. \quad (9)$$

Minimization with respect to  $\theta, \Delta\phi$  gives  $\Delta\phi = \cos^{-1}(1/\rho)$  (it does not depend on  $h$ ), and

$$M_{Umb} = \cos\theta = \frac{h\rho}{2(\rho+1)^2}, \quad (10)$$

$$\epsilon_{Umb} = -\frac{1}{\rho} - \frac{\rho}{2} - \frac{h^2\rho}{4(\rho+1)^2}. \quad (11)$$

The umbrella structure exists for  $\rho > 1$  and  $h < h_{max} = 2(\rho+1)^2/\rho$ , has energy lower than the spin-flop one, and turns into the spin-flop structure at  $\rho = 1$ . At  $h = h_{max}$  it becomes the spin-flip structure. Both phase transitions are of the second order. In Fig. 3 and Fig. 4 numerically calculated umbrella structures for  $(\rho, h) = (1.5, 3)$  and  $(1.2, 3)$  respectively are presented (See section IV below for details).

The phase diagram of the classical isotropic SSL is shown in Fig. 5. The solid lines mark the lines of the second order phase transitions. For  $\rho < 1$  SSL behaves exactly like a regular Neel antiferromagnet, while for  $\rho > 1$  the spin-flop phase is replaced by the umbrella phase. The dotted line denotes the special degenerate case  $\rho = 2$ . Magnetization curve  $M(h)$  are linear until

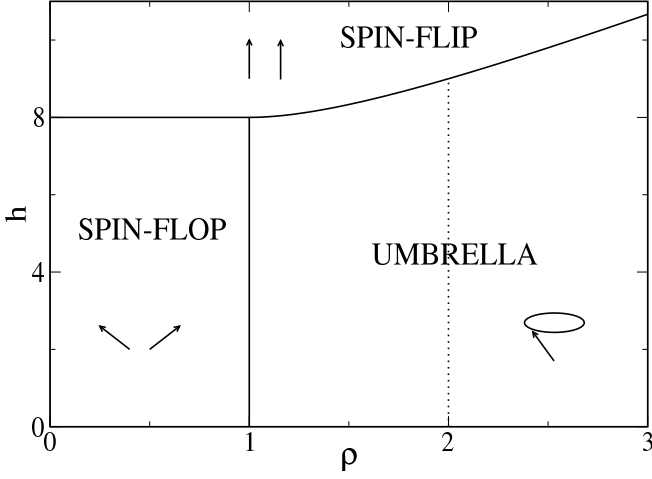


FIG. 5.  $T = 0$  phase diagram of the classical SSL. The solid lines correspond to second order phase transitions. The dotted line mark the special degenerate case  $J_2/J_1 = 2$ .

saturation, and there is no magnetization plateaus for the isotropic Heisenberg SSL. Note that the  $1/3$  pseudo-plateau observed in Ref. 13 was a finite-temperature effect. The phase diagram in Fig. 5 has been constructed by comparing energies of different spin structures introduced in this section and selecting the one with the lowest energy for a given  $(\rho, h)$ . In order to prove that this phase diagram is indeed correct, we have to show that there are no other spin structures with lower energy. This is done in the next section.

### III. EXACT GROUND STATE

In order to prove that the three spin structures introduced in the previous section (spin-flop, spin-flip and umbrella) are indeed the ground state structures for respective  $(\rho, h)$  we use the method of decomposing the Hamiltonian into overlapping elementary clusters, which has been used previously in, e.g., Refs. 1, 13, and 19

$$\tilde{\mathcal{H}} = \sum_{\Delta} \mathcal{H}_{\Delta}. \quad (12)$$

For SSL such elementary cluster has the shape of the right triangle, highlighted in red in Fig. 1. Each triangle includes one spin  $\mathbf{S}_0$  at the right angle, two spins ( $\mathbf{S}_1$  and  $\mathbf{S}_2$ ) at the  $45^\circ$  angles; two  $J_1$  bonds, and one  $J_2$  bond shared by two triangles. The number of triangles on the lattice is the same as the number of lattice sites, as each triangle includes 3 spins and each spin is a part of 3 triangles. The Hamiltonian of a triangle is

$$\mathcal{H}_{\Delta} = \mathbf{S}_0 (\mathbf{S}_1 + \mathbf{S}_2) + \frac{\rho}{2} \mathbf{S}_1 \mathbf{S}_2 - \mathbf{h} \left[ \alpha \mathbf{S}_0 + \frac{1-\alpha}{2} (\mathbf{S}_1 + \mathbf{S}_2) \right], \quad (13)$$

where  $\alpha$  is an arbitrary real number. It corresponds to an arbitrary way in which the term  $-\mathbf{h}\mathbf{S}_i$  of the origi-

nal Hamiltonian can be divided between three different triangles which include the site  $\mathbf{S}_i$ . The triangle Hamiltonian is invariant under three basic symmetry operations: simultaneous rotation of all spins around  $z$  axis, reflection of all spins in  $xz$  plane, and interchange  $\mathbf{S}_1 \leftrightarrow \mathbf{S}_2$ , where  $z$ -axis is parallel to  $\mathbf{h}$ . These operations generate a symmetry group, which also includes such operations as reflection in  $yz$  plane (or any other plane containing  $z$  axis) and inversion of the  $xy$  components of all spins  $\mathbf{S}_i^x \rightarrow -\mathbf{S}_i^x$ ,  $\mathbf{S}_i^y \rightarrow -\mathbf{S}_i^y$  ( $i = 0, 1, 2$ ). This symmetry leads to the degeneracy of most energy levels  $\epsilon(\alpha, \mathbf{S}_0, \mathbf{S}_1, \mathbf{S}_2)$ , as the only configurations invariant under the symmetry group of  $\mathcal{H}_{\Delta}$  are collinear ones with  $\mathbf{S}_0 = \pm \mathbf{z}$  and  $\mathbf{S}_1 = \mathbf{S}_2 = \pm \mathbf{z}$ . At the special point  $\rho = 2$  there is an additional symmetry operation  $\mathbf{S}_0 \leftrightarrow \mathbf{S}_1$  (or  $\mathbf{S}_0 \leftrightarrow \mathbf{S}_2$ ).

The triangle Hamiltonian has an  $\alpha$ -dependent ground state energy  $\epsilon_0(\alpha)$ , thus for every possible configuration of three unit vectors  $\mathbf{S}_0, \mathbf{S}_1$ , and  $\mathbf{S}_2$  the inequality

$$\epsilon_{\Delta}(\mathbf{S}_0, \mathbf{S}_1, \mathbf{S}_2, \alpha) \geq \epsilon_0(\alpha) \quad (14)$$

holds true. The equality is achieved for a possibly degenerate ground state configuration of the triangle Hamiltonian. There is also an inequality for the lattice energy, which holds true for all values of  $\alpha$

$$N\epsilon\{\mathbf{S}_i\} = \sum_{\Delta} \epsilon_{\Delta} \geq \sum_{\Delta} \epsilon_0(\alpha) = N\epsilon_0(\alpha), \quad (15)$$

or  $\epsilon\{\mathbf{S}_i\} \geq \epsilon_0(\alpha)$ , where  $N$  is the number of lattice sites, and  $\epsilon\{\mathbf{S}_i\}$  is the energy per site. The equality here is possible only for a spin structure  $\{\mathbf{S}_i\}$  that minimizes the energy of each triangle simultaneously. Here and in the following we use the word "structure" for spin structures  $\{\mathbf{S}_i\}$  on the lattice, and the word "configuration" for configurations  $\mathbf{S}_0, \mathbf{S}_1$ , and  $\mathbf{S}_2$  of the three spins of a triangle. According to (15), for every other spin structure  $\{\mathbf{S}'_i\}$  one can write an inequality  $\epsilon\{\mathbf{S}'_i\} \geq \epsilon_0(\alpha) = \epsilon\{\mathbf{S}_i\}$ , which proves that the structure  $\{\mathbf{S}_i\}$  is indeed the ground state of the lattice Hamiltonian (2), or, in general, one of the degenerate ground state structures. In other words, in order to find the ground state of the lattice Hamiltonian (2) for a given  $(\rho, h)$ , we have to construct a lattice spin structure  $\{\mathbf{S}_i\}$  from the ground state configuration  $(\mathbf{S}_0, \mathbf{S}_1, \mathbf{S}_2)$  of a triangle (let us call it "brick"), or from a set of such bricks in case of degeneracy. In case of a degenerate ground state, it is important to note that any possible lattice structure constructed from bricks is a ground state structure, and, vice versa, any possible ground state structure can be constructed from bricks (which can be seen from the fact that for any ground state structure the energy of each triangle is equal to  $\epsilon_0$ ).

The question is whether it is possible to construct a lattice structure from a given set of bricks, which includes all possible realization of the degenerate ground state of  $\mathcal{H}_{\Delta}$ , spawned by the symmetry group of  $\mathcal{H}_{\Delta}$ . The problem is not trivial, since each spin is a part of three different triangles, so the bricks must match each other perfectly. This is obviously not possible for arbitrary  $\alpha$ ,

	Energy	Domain
Flip	$2 + \rho/2 \mp h$	
Neel	$-2 + \rho/2 \mp h(1 - 2\alpha)$	
Dimer	$-\rho/2 \mp h\alpha$	
Umb	$-1/\rho - \rho/2 - \frac{h^2\rho}{4(\rho+1)^2}$	$\rho \geq 1, h < \frac{2(\rho+1)^2}{\rho}$
$Y_1$	$-\frac{1}{\rho} - \frac{\rho}{2} + h\left(\alpha - \frac{\alpha'}{\rho}\right) - \frac{\alpha'^2 h^2}{4\rho}$	$\frac{\alpha' h}{2} < \rho - 1$
$Y_2$	$-\frac{1}{\rho} - \frac{\rho}{2} - h\left(\alpha - \frac{\alpha'}{\rho}\right) - \frac{\alpha'^2 h^2}{4\rho}$	$1 - \rho < \frac{\alpha' h}{2} < 1 + \rho$
Flop	$\frac{\rho}{2} - \frac{\alpha(1-\alpha)h^2}{4} - \left(\frac{\alpha'}{\alpha} + \frac{\alpha}{\alpha'}\right)$	$h < \frac{2}{\alpha\alpha'}$

TABLE I. Energies  $\epsilon(\alpha)$  and domains of existence of different configurations of a triangle, which are energy extrema of  $\mathcal{H}_\Delta$ . We use the definition  $\alpha' \equiv 1 - \alpha$ . The umbrella configuration is only defined for  $\alpha = 1/(\rho + 1)$ .

however, as we are going to see below, such construction can indeed be performed for the right choice of  $\alpha$ . The required values are  $\alpha = 1/2$  for  $\rho \leq 1$ , and  $\alpha = 1/(\rho + 1)$  for  $\rho > 1$ , respectively. For these values of  $\alpha$  we can construct the spin-flop, spin-flip and umbrella structures from the ground state configurations of  $\epsilon_\Delta$  and confirm the phase diagram of Fig. 5. Contrary to the case of the Ising SSL<sup>19</sup>, the phase diagram of the classical Heisenberg SSL does not have the convexity property, so the search for ground state must be performed for arbitrary  $(\rho, h)$ , rather than for a finite number of special points.

For simplicity we assume that  $h > 0$ , so that the field  $\mathbf{h}$  provides a fixed direction  $\mathbf{z}$ . The rather trivial case  $h = 0$  (solved in Ref. 1 by the same method) has been discussed in the previous section. Let us find all possible steady states (energy extrema) of the triangle Hamiltonian (13) and their energies (listed in Table I). They can be found from the system of three vector equations

$$\frac{\partial}{\partial \mathbf{S}_j} \left( \mathcal{H}_\Delta - \frac{1}{2} \sum_i \xi_i \mathbf{S}_i \mathbf{S}_i \right) = 0, \quad i, j = 0, 1, 2 \quad (16)$$

for the three unit vectors  $\mathbf{S}_0, \mathbf{S}_1, \mathbf{S}_2$ :

$$\frac{\partial \mathcal{H}_\Delta}{\partial \mathbf{S}_1} = \mathbf{S}_0 + \frac{\rho}{2} \mathbf{S}_2 - \frac{1 - \alpha}{2} \mathbf{h} = \xi_1 \mathbf{S}_1, \quad (17)$$

$$\frac{\partial \mathcal{H}_\Delta}{\partial \mathbf{S}_2} = \mathbf{S}_0 + \frac{\rho}{2} \mathbf{S}_1 - \frac{1 - \alpha}{2} \mathbf{h} = \xi_2 \mathbf{S}_2, \quad (18)$$

$$\frac{\partial \mathcal{H}_\Delta}{\partial \mathbf{S}_0} = \mathbf{S}_1 + \mathbf{S}_2 - \alpha \mathbf{h} = \xi_0 \mathbf{S}_0, \quad (19)$$

where  $\xi_i$  are the three real Lagrange multipliers used to enforce the conditions  $\mathbf{S}_i \mathbf{S}_i = 1$ . They are nonpositive for local energy minima, and nonnegative for local maxima.

First, let us consider collinear ( $\mathbf{S}_i = \pm \mathbf{z}$ ) solutions of Eqs. (17)–(19). Any collinear configuration is a solution. The energies of two spin-flip-like configuration ( $\mathbf{S}_i = \pm \mathbf{z}$ ) are  $\epsilon_{Flip1,2} = 2 + \rho/2 \mp h$  and do not depend on  $\alpha$ . The two Neel-like configurations ( $\mathbf{S}_1 = \mathbf{S}_2 = -\mathbf{S}_0 = \pm \mathbf{z}$ ) have

energies  $\epsilon_{Neel1,2} = -2 + \rho/2 \mp h(1 - 2\alpha)$ . Finally, the two dimer-like configurations ( $\mathbf{S}_1 = -\mathbf{S}_2 = \mathbf{z}, \mathbf{S}_0 = \pm \mathbf{z}$ ) have energies  $\epsilon_{Dimer1,2} = -\rho/2 \mp h\alpha$ . Now let us find all noncollinear solutions of Eqs. (17)–(19). Subtracting first two equations gives

$$\mathbf{S}_1 \left( \xi_1 + \frac{\rho}{2} \right) = \mathbf{S}_2 \left( \xi_2 + \frac{\rho}{2} \right). \quad (20)$$

It means that either  $\mathbf{S}_1$  and  $\mathbf{S}_2$  are collinear, or that both expressions in parentheses are equal to zero. There are 3 possible cases

**Case 1:**  $\xi_1 = \xi_2 = -\rho/2$ ,

**Case 2:**  $\mathbf{S}_1 = -\mathbf{S}_2$ ,

**Case 3:**  $\mathbf{S}_1 = \mathbf{S}_2$ .

Below we shall consider all 3 cases in detail.

**Case 1:**  $\xi_1 = \xi_2 = -\rho/2$ . We introduce a new variable  $\mathbf{S} \equiv (\mathbf{S}_1 + \mathbf{S}_2)/2$ , and note that  $0 \leq |\mathbf{S}| \leq 1$ , but  $|\mathbf{S}_0| = 1$ . The equations (17)–(19) become

$$\mathbf{S}_0 + \rho \mathbf{S} = \mathbf{h}(1 - \alpha)/2, \quad (21)$$

$$2\mathbf{S} - \alpha \mathbf{h} = \xi_0 \mathbf{S}_0. \quad (22)$$

Excluding  $\mathbf{S}_0$  gives

$$\mathbf{S}(2 + \xi_0 \rho) = \mathbf{h}[\alpha + \xi_0(1 - \alpha)/2]. \quad (23)$$

There are again two possible cases.

**Case 1.1:**  $2 + \xi_0 \rho = \alpha + \xi_0(1 - \alpha)/2 = 0$ . This is only possible for  $\alpha = 1/(\rho + 1)$ , which shows that it is indeed the correct value of  $\alpha$  for  $\rho > 1$ , since no other value of  $\alpha$  can produce the umbrella phase. For this value of  $\alpha$  there is an entire family of the degenerate "umbrella-like" solutions of the form

$$\mathbf{S}_0 + \rho \mathbf{S} = \frac{\rho \mathbf{h}}{2(\rho + 1)} \quad (24)$$

for  $h < h_{max} = 2(\rho + 1)^2/\rho$  with the energy

$$\epsilon_{Umb} = -\frac{1}{\rho} - \frac{\rho}{2} - \frac{h^2 \rho}{4(\rho + 1)^2}. \quad (25)$$

For case  $\rho = 2$ , this degeneracy is preserved at the lattice level<sup>13</sup>, namely, every configuration with  $\mathbf{S}_0 + \mathbf{S}_1 + \mathbf{S}_2 = \mathbf{h}/3$  can form a lattice structure consisting of three types of sites (for example, ordered as in Fig. 2, lower right), since  $\mathbf{S}_0, \mathbf{S}_1$ , and  $\mathbf{S}_2$  can be interchanged freely. In particular, the UUD structure can be realized at a single point  $(\rho, h) = (2, 3)$ . For  $\rho \neq 2$  the requirement of bricks matching each other partly lifts the degeneracy and leads to the umbrella structure, for which  $\mathbf{S}_i \mathbf{h} = \cos \theta$  is equal for all spins. For  $\alpha = 1/2, \rho < 1$  there is no solutions of this kind.

**Case 1.2:**  $\mathbf{S}$ ,  $\mathbf{S}_0$  and  $\mathbf{h}$  are collinear (but  $\mathbf{S}_{1,2}$  and  $\mathbf{h}$  are not). This gives up to two Y-like configurations, with  $\mathbf{S} \parallel \mathbf{z}$  and  $\mathbf{S}_0 = \pm \mathbf{z}$ . The  $Y_1$  configuration with  $\mathbf{S}_0 = -\mathbf{z}$  has the energy

$$\epsilon_{Y_1}(\alpha) = -\frac{1}{\rho} - \frac{\rho}{2} + h \left( \alpha - \frac{1-\alpha}{\rho} \right) - \frac{(1-\alpha)^2 h^2}{4\rho} \quad (26)$$

and it exists for  $h < 2(\rho-1)/(1-\alpha)$ . The  $Y_2$  configuration with  $\mathbf{S}_0 = +\mathbf{z}$  has the energy

$$\epsilon_{Y_2}(\alpha) = -\frac{1}{\rho} - \frac{\rho}{2} - h \left( \alpha - \frac{1-\alpha}{\rho} \right) - \frac{(1-\alpha)^2 h^2}{4\rho} \quad (27)$$

and it exists for  $1-\rho < (1-\alpha)h/2 < 1+\rho$ .

For  $\alpha = 1/(\rho+1)$ ,  $\rho > 1$  the  $Y_{1,2}$  solutions are just two special cases of the umbrella-like solution introduced above. For  $\alpha = 1/2$ ,  $\rho \leq 1$  there is a single  $Y_2$  solution with the energy

$$\epsilon_{Y_2} = -\frac{1}{\rho} - \frac{\rho}{2} - \frac{h(\rho-1)}{2\rho} - \frac{h^2}{4\rho}. \quad (28)$$

**Case 2:**  $\mathbf{S}_1 = -\mathbf{S}_2$ . The dimer-like collinear solutions belong to this case, but there are no noncollinear solutions.

**Case 3:**  $\mathbf{S}_1 = \mathbf{S}_2 = \mathbf{S}$  and  $\xi_1 = \xi_2 = \xi$ . The equations (17)–(19) take the form

$$\mathbf{S}_0 + \left( \frac{\rho}{2} - \xi \right) \mathbf{S} = \frac{1-\alpha}{2} \mathbf{h} \quad (29)$$

$$2\mathbf{S} - \alpha \mathbf{h} = \xi_0 \mathbf{S}_0, \quad (30)$$

or, after excluding  $\mathbf{S}_0$ ,

$$\mathbf{h} \left[ \alpha + \frac{\xi_0(1-\alpha)}{2} \right] = \mathbf{S} \left[ 2 - \xi_0 \left( \xi - \frac{\rho}{2} \right) \right]. \quad (31)$$

As before, it can mean either that  $\mathbf{S}$  is collinear with  $\mathbf{h}$  (which leads to collinear spin-flip and Neel-like solutions), or that both expressions in the square brackets are equal to zero, which leads to

$$\xi_0 = -\frac{2\alpha}{1-\alpha}, \quad \xi = \frac{\rho}{2} - \frac{1-\alpha}{\alpha}, \quad (32)$$

and

$$\mathbf{S} + \mathbf{S}_0 \frac{\alpha}{1-\alpha} = \frac{\alpha}{2} \mathbf{h}, \quad (33)$$

which is the spin-flop-like solution with the energy

$$\epsilon_{Flop}(\alpha) = \frac{\rho}{2} - \frac{\alpha(1-\alpha)}{4} h^2 - \frac{1-\alpha}{\alpha} - \frac{\alpha}{1-\alpha}. \quad (34)$$

It exists for  $h < 2/(\alpha(1-\alpha))$ . For  $\alpha = 1/(\rho+1)$ ,  $\rho > 1$  this is again a special case of the umbrella-like solution. For  $\alpha = 1/2$ ,  $\rho \leq 1$  this is the spin-flop solution ( $\mathbf{S} + \mathbf{S}_0 = \mathbf{h}/4$ ) with the energy  $\epsilon_{Flop} = -2 + \rho/2 - h^2/16$ . The spin-flop-like bricks only match if  $\mathbf{S}\mathbf{h} = \mathbf{S}_0\mathbf{h}$ , i.e. that all spins

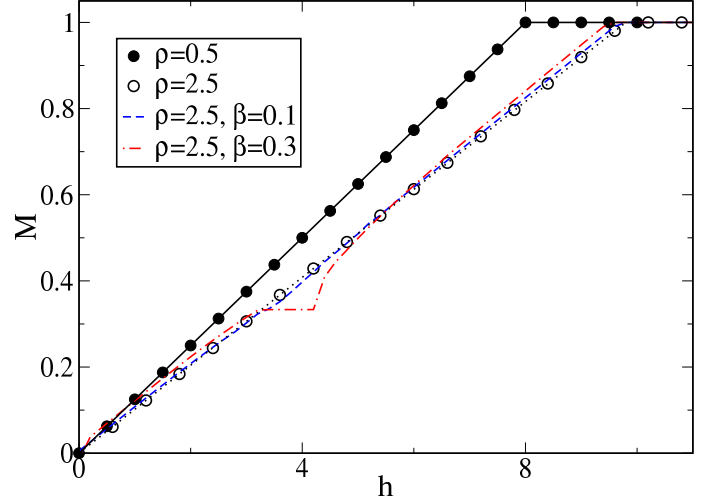


FIG. 6. (Color online) Magnetization curves  $M(h)$  for the classical SSL.  $\rho = 0.5$ , no anisotropy: exact result (solid black line), numerical data (solid circles).  $\rho = 2.5$ , no anisotropy: exact result (dotted black line), numerical data (empty circles).  $\rho = 2.5$ , with anisotropy:  $\beta = 0.1$  (blue dashed line),  $\beta = 0.3$  (red dash-dot curve). All numerical calculations have been performed on the  $12 \times 12$  lattice with periodic boundary conditions.

are tilted by the same angle  $\theta'$  relative to the  $xy$ -plane. This condition gives  $\alpha = 1/2$  as the only value of  $\alpha$  for which the construction of the spin-flop lattice structure is possible.

Some of the configurations corresponding to the energy extrema of  $\mathcal{H}_\Delta$  do not match and thus cannot form a spin structure on the lattice. The ones that do are: spin-flop and Neel (for  $\alpha = 1/2$ ), umbrella-like (for  $\alpha = 1/(\rho+1)$ ), dimer (for  $\alpha = 0$ ), and spin-flip (for any  $\alpha$ ). The direct comparison of their energies (listed in Table I) for respective values of  $\alpha$  shows that spin-flop, umbrella-like and spin-flip solutions indeed minimize the triangle Hamiltonian (13) in the three respective regions of Fig. 5. The Neel structure is only realized for  $h = 0$ ,  $\rho \leq 1$ . The dimer structure does not exist for isotropic classical Heisenberg SSL. This confirms the phase diagram shown in Fig. 5.

#### IV. NUMERICAL SIMULATIONS AND THE EFFECT OF ANISOTROPY

In order to give an independent check of our exact results we performed a series of numerical simulations, calculating the ground state of lattice Hamiltonian  $\tilde{\mathcal{H}}$  for different values of  $\rho$ ,  $h$ . We have also examined the effect of uniaxial anisotropy by adding the term

$$\mathcal{H}_A = \frac{B}{2} \sum_i (1 - (S_i^z)^2) \quad (35)$$

to the Hamiltonian  $\mathcal{H}$ , or, equivalently, adding the term

$$\tilde{\mathcal{H}}_A = \frac{\beta}{2} \sum_i (1 - (S_i^z)^2) \quad (36)$$

to  $\tilde{\mathcal{H}}$ , where  $\beta \equiv B/J_1$  is the anisotropy constant.

The minimum of  $\tilde{\mathcal{H}}$  was found by a discrete micromagnetic simulation with only the Gilbert damping term included. We considered the system of equations

$$\frac{d\mathbf{S}_i}{dt} = -\lambda \left[ \frac{\partial \tilde{\mathcal{H}}}{\partial \mathbf{S}_i} - \mathbf{S}_i \left( \mathbf{S}_i \cdot \frac{\partial \tilde{\mathcal{H}}}{\partial \mathbf{S}_i} \right) \right], \quad (37)$$

where  $\lambda > 0$  is the damping parameter, for each spin  $\mathbf{S}_i$  of the lattice; and solved it using the first-order Runge-Kutta method in spherical coordinates with our own computer code. This method decreases the energy of the system on each step (provided that  $\lambda$  is small enough) eventually finding a (local) minimum. It can be viewed as a variation of the steepest descend method. Unlike previously used Monte Carlo methods, our method looks for the ground state of the system avoiding any finite-temperature effects. We have used cells of different size ( $6 \times 6$ ,  $12 \times 12$ , and  $24 \times 24$ ) with periodic boundary condition. In order to minimize the probability of finding a local energy minimum instead of the ground state, each simulations was performed 50 times with different random initial conditions, and the result with the lowest energy was chosen.

A number of simulations for different values of  $\rho$ ,  $h$  have been performed. Our results fully confirm the phase diagram of Fig. 5, in particular, the second order phase transitions and the additional degeneracy for  $\rho = 2$  are clearly seen in our calculations. We have also applied the same method to the triangle Hamiltonian  $\mathcal{H}_\Delta$  and checked numerically the validity of the results of the previous section. Two typical magnetization curves  $M(h)$  are presented in Fig. 6 for  $\rho = 0.5$  and  $\rho = 2.5$ . The numerical results are plotted as circles in this figure, while the analytical formulae (4)–(10) are presented as lines. For  $\rho = 0.5$  the system goes through the sequence of the Neel–spin-flop–spin-flip structures, all of them being periodic with 4 atoms per unit cell, exactly as predicted by our analytical treatment above. The  $M(h)$  curves in fact do not depend on  $\rho$  at all as long as  $\rho \leq 1$ . For  $\rho > 1$  the ground state is the umbrella structure, which is in general incommensurate with the lattice. The numerical calculations with a finite lattice size cannot reproduce this phase exactly, of course, but as long as the lattice size is  $6 \times 6$  or larger, the resulting umbrella-like phase has magnetization and energy very close to the values given by Eqs. (10), (11). Even for the  $6 \times 6$  lattice the relative difference between theoretical and calculated  $M$  is only about  $9 \times 10^{-4}$ , a difference too small to be seen in the scale of Fig. 6. Examples of such umbrella structures with periodicity forced by the lattice size are presented in Fig. 3 and Fig. 4 for  $(\rho, h) = (1.5, 3)$  and  $(1.2, 3)$  respectively.

If the magnetic anisotropy  $\beta$  is switched on, the single UUD point  $(\rho, h) = (2, 3)$  expands into a finite region of the UUD phase. The  $M(h)$  curves for  $\rho \neq 2$  first get a noticeable kink at around  $M = 1/3$  (Fig. 6, dashed blue curve), which eventually turns into the  $M = 1/3$  UUD plateau when the anisotropy constant is increased (Fig. 6, dashed-dot red curve). For  $\rho = 2$  the  $M = 1/3$  step appears for any finite value of  $\beta$ . Our  $M(h)$  curves are very similar to the  $M(h)$  curves of Ref. 14, which were obtained using Monte Carlo method for  $\rho = 2$ . However, we observed the onset of the  $1/3$  plateau at a finite value of  $\beta$ , which was not seen in Ref. 14 due to the choice of a non-arbitrary point  $\rho = 2$ . No plateaus other than  $1/3$  appear in our calculations.

It is interesting to compare the different physics of Ising and classical Heisenberg SSL. The Ising SSL allows for collinear structures only, and its zero-temperature  $M(h)$  curves consist of vertical and horizontal segments only (plateaus and first order phase transition). In contrast, magnetization curves for isotropic Heisenberg SSL are linear until saturation thanks to noncollinear spin-flop and umbrella structures. The anisotropic Heisenberg SSL combines features of both Ising and Heisenberg models. Its magnetization curves  $M(h)$  can include both horizontal steps (corresponding to collinear spin structures) and inclined regions (corresponding to noncollinear structures). While the Ising approach might be sufficient for  $\text{TmB}_4$ , both types of regions are clearly seen experimentally in  $\text{HoB}_4$ . In fact, the experimental  $M(h)$  curve for  $\text{HoB}_4$  (Ref. 12) is remarkably similar to our  $M(h)$  curve for  $\rho = 2.5$ ,  $\beta = 0.3$  (dashed-dot red curve in Fig. 6). The next logical step in the study of classical Heisenberg SSL would be determining of the phase diagram of the classical Heisenberg SSL with easy-axis anisotropy. This problem is, however, beyond the scope of the present paper and will be addressed in our future research.

## V. CONCLUSION

We have determined analytically the exact ground state of the classical Heisenberg SSL in the external field  $h$  and presented the phase diagram of this model in the  $(\rho, h)$  plane. The phase diagram includes the spin-flop phase for  $\rho \leq 1$ , the umbrella phase for  $\rho > 1$ , and the spin-flip phase for sufficiently large  $h$ . The phase transitions between these three phases are of the second order. The zero-temperature magnetization curves  $M(h)$  are linear until saturation with no features. For  $\rho = 2$  there is an additional degeneracy and an infinite number of spin structures which share the energy and magnetization with the umbrella one. In particular, UUD structure can be realized at a single point  $(\rho, h) = (2, 3)$ .

The effect of the easy-axis uniaxial anisotropy on  $M(h)$  curves has been examined by numerical micromagnetic simulation. The anisotropy leads to the onset of the  $M = 1/3$  UUD plateau at a certain finite value of the anisotropy constant  $\beta$  for  $\rho \neq 2$  (and at  $\beta = 0$  for  $\rho = 2$ ).



Our results demonstrate the existence of both collinear (steps of the  $M(h)$  curve) and noncollinear (inclined parts of the  $M(h)$  curve) spin structures for anisotropic Heisenberg SSL. The results explain the magnetization curve of  $\text{HoB}_4$ , while the  $M(h)$  curves of  $\text{TmB}_4$  are more Ising-like in nature, and cannot be explained without introducing

additional interactions into the model.

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